RESEARCH PAPER

Synthesis for the Different Fragrance and Their application

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Abstract—*Fragrance ingredients are volatile organic molecules whose commercial value depends on a combination of odor quality, stability, safety and production cost. This review surveys how the principal classes of fragrance molecules—terpenoids, aromatic aldehydes and lactones, esters, musks and amber-type compounds—are obtained, from botanical extraction to catalytic, enzymatic and fermentative synthesis, and relates each route to its end use. Three analyses go beyond a narrative summary. First, a volatility map of sixteen representative odorants links molecular weight and boiling point to the familiar top-, heart- and base-note scheme. Second, atom economy is recomputed from balanced equations for eight industrially relevant transformations; catalytic addition and hydrogenation steps reach 100 %, whereas condensation and acylation routes fall to 65–71 %. Third, a five-criterion qualitative scoring of production strategies shows that no single approach dominates, and that biocatalysis and asymmetric catalysis complement each other in stereocontrol and waste minimisation. Application requirements, allergen and environmental regulation through 2023, and the emerging role of data-driven odor prediction are discussed, and open research problems are identified.*

Index Terms—*fragrance synthesis, terpenoids, vanillin, menthol, musks, biocatalysis, atom economy, green chemistry, perfumery applications*

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Introduction

Fragrance ingredients are small, volatile organic molecules, typically with molecular weights between about 100 and 300 g mol^{-1}, that interact with the human olfactory system and form the basis of perfumery, cosmetics, household products and flavours [1], [2]. For most of history, the perfumer's palette was limited to what could be pressed, distilled or extracted from plants and animals. The first laboratory preparation of coumarin by Perkin in 1868 [3] opened the way to a palette that is now dominated by molecules that are made, not harvested, and over the following century organic synthesis supplied odorants that nature produces only in trace amounts or not at all [4], [5].

The field now faces several simultaneous pressures. Consumers and brand owners ask for "natural" and bio-based ingredients; regulators have tightened rules on allergens, persistent compounds and polymer microparticles [6], [7], [8]; and manufacturers must reduce waste and energy use while keeping the stereochemical purity that governs odor. At the same time, biocatalysis, fermentation and flow processing have matured to a point where they compete with classical routes [9], [10].

Excellent monographs describe fragrance chemistry in depth [2], [11], [12], and landmark reviews summarise progress up to the early 2000s [4], [5]. What is missing is a compact comparison that places traditional organic routes, biotechnological routes and sustainability metrics side by side. This article makes three contributions: (i) a volatility map that connects physical properties to perfume structure; (ii) a recomputation of atom economy for eight representative transformations, using balanced equations; and (iii) a transparent, criterion-based comparison of five production strategies. Sections II–III cover odor fundamentals and natural sourcing, Section IV the synthesis of the main compound families, Section V biotechnological and green routes, Section VI the comparative assessment, and Sections VII–IX applications, regulation and outlook.

II. Odor Fundamentals and Classification

A. Structure–Odor Relationships

Odor arises when volatile molecules bind to olfactory receptors in the nasal epithelium. Humans possess roughly four hundred functional receptor genes, and each odorant activates a characteristic combination of receptors rather than a single one, which allows a limited receptor repertoire to discriminate a very large number of smells [13], [14]. A consequence is that odor does not follow simple structural rules. Enantiomers smell different—(*R*)-carvone is spearmint-like and (*S*)-carvone caraway-like—and a small change in a functional group transforms a floral note into a fruity or animalic one [1]. Fragrance chemists rely on empirical families, on gas chromatography–olfactometry to link chemical peaks to perceived odor [15], and increasingly on machine-learning models trained on panel data. Models developed in a 2017 crowd-sourced challenge showed that perceptual ratings are predicted from molecular features [16], and a graph neural network "principal odor map" reported in 2023 matched or exceeded the typical individual panelist in describing odors [17].

B. Volatility and the Perfume Pyramid

Perfumers arrange ingredients by evaporation rate into top, heart and base notes. Volatility depends on molecular size, polarity and hydrogen bonding, and boiling point is a convenient proxy. Fig. 1 plots sixteen widely used odorants. Light terpene hydrocarbons and small esters such as α-pinene, limonene and isoamyl acetate fall in the top-note region (boiling point below about 200 °C), whereas the heavier phenolic and lactone compounds vanillin and coumarin sit in the base region (above about 250 °C). Terpenoid alcohols and many floral materials such as linalool, geraniol and 2-phenylethanol occupy the heart. The band limits are conventions rather than physical thresholds,

and the plot also shows that molecular weight alone is a poor predictor: hydrogen-bonding aromatics boil far higher than terpenes of equal mass.

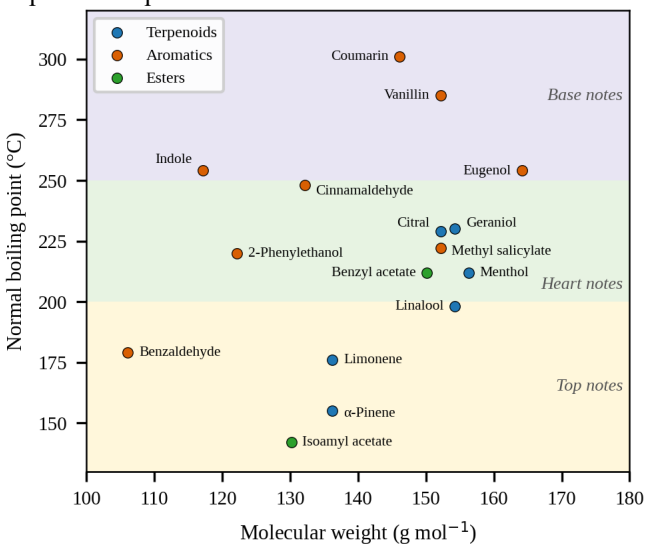


Fig. 1. Volatility map of sixteen representative odorants. Shaded bands show the conventional top-, heart- and base-note regions (approximate limits). Molecular weights were calculated from molecular formulas; boiling points are standard handbook values rounded to the nearest degree [2].

III. Natural Sourcing and Extraction

Botanical raw materials are important because they supply complex mixtures and natural enantiomers. Classical operations include steam distillation and hydrodistillation of leaves, woods and flowers, cold expression of citrus peel, and solvent extraction of delicate flowers to give concretes and absolutes [11], [2]. Their drawbacks are seasonal and geographic variation, low yield and, for solvent processes, residual solvent. Greener alternatives address these issues. Supercritical CO_2 extracts and fractionates oils at low temperature without solvent residue [18], and solvent-free microwave extraction shortens processing time compared with conventional hydrodistillation [19]. The principles that guide such "green extraction" have been formalised in the literature [20].

Two natural streams also act as chemical feedstocks. Citrus processing yields large volumes of limonene, which is used directly and as a building block for further transformations [21]. Turpentine from pine—obtained as a by-product of wood pulping—supplies α- and β-pinene, which are the starting materials for many terpenoid odorants, including linalool and its esters [22], [2]. Semisynthesis from such renewable streams is a central strategy in industrial fragrance chemistry (Fig. 2).

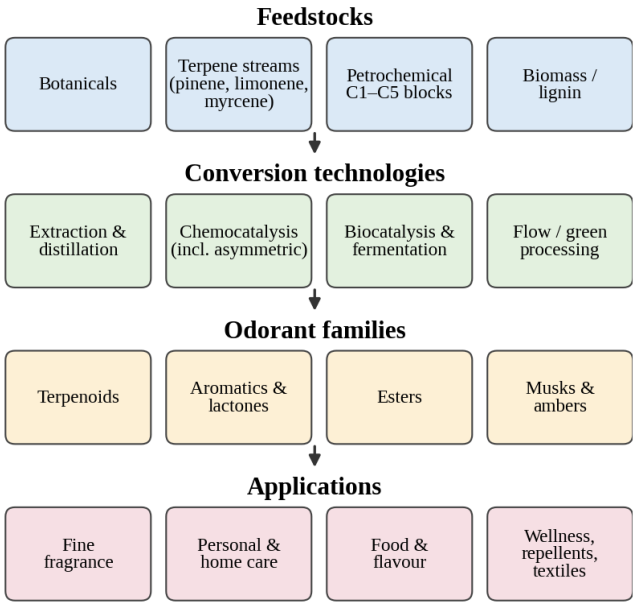


Fig. 2. Conceptual map of fragrance production: feedstocks, conversion technologies, odorant families and application sectors discussed in this review.

IV. Synthesis of Principal Fragrance Families

Table I lists eleven commercially important odorants with their formulas, molecular weights and principal industrial routes, and Fig. 3 outlines three of the best-documented sequences. The routes illustrate recurring design themes: assembling terpenoid skeletons from small isoprenoid units, controlling stereochemistry with catalysts, and building aromatic or macrocyclic frameworks by classical named reactions.

TABLE I
Selected fragrance molecules and principal synthetic routes

Compound (formula, *M*)	Odor	Principal industrial route	Typical use
Linalool ($C_{10}H_{18}O$, 154.25)	floral, woody	α-Pinene → pinane → hydroperoxide → pinanol → pyrolysis; or methylheptenone + acetylene, then partial hydrogenation	Perfumery, personal care, intermediate
Citral ($C_{10}H_{16}O$, 152.24)	lemon	Prenol/prenal acetal; Claisen and Cope rearrangements	Citrus notes, precursor of ionones
(−)-Menthol ($C_{10}H_{20}O$, 156.27)	cooling, mint	Asymmetric Rh-BINAP isomerisation of geranyl-amine; or thymol hydrogenation	Oral care, confectionery, topicals

Compound (formula, *M*)	Odor	Principal industrial route	Typical use
Vanillin ($C_8H_8O_3$, 152.15)	vanilla	Guaiacol + glyoxylic acid; lignin oxidation; ferulic acid bioconversion	Food, fine fragrance
Coumarin ($C_9H_6O_2$, 146.14)	sweet, hay	Perkin reaction of salicylaldehyde	Fougère accords
2-Phenylethanol ($C_8H_{10}O$, 122.17)	rose	Friedel–Crafts with ethylene oxide; styrene oxide hydrogenation; yeast fermentation	Floral bases, soaps
Benzyl acetate ($C_9H_{10}O_2$, 150.18)	jasmine, fruity	Esterification of benzyl alcohol	Floral compositions
Methyl dihydrojasmonate ($C_{13}H_{22}O_3$, 226.32)	transparent jasmine	Aldol condensation of cyclopentanone and pentanal; Michael addition; decarboxylation	Fine fragrance
(−)-Ambrox ($C_{16}H_{28}O$, 236.40)	ambergris	Sclareol → sclareolide → diol → cyclisation; or homofarnesol cyclisation	Base note, fixative
Galaxolide ($C_{18}H_{26}O$, 258.40)	sweet musk	Pentamethylindane + propylene oxide; formaldehyde cyclisation	Detergents, personal care
Ethylene brassylate ($C_{15}H_{26}O_4$, 270.37)	musk	Brassylic acid + ethylene glycol; depolymerisation	Fine and household

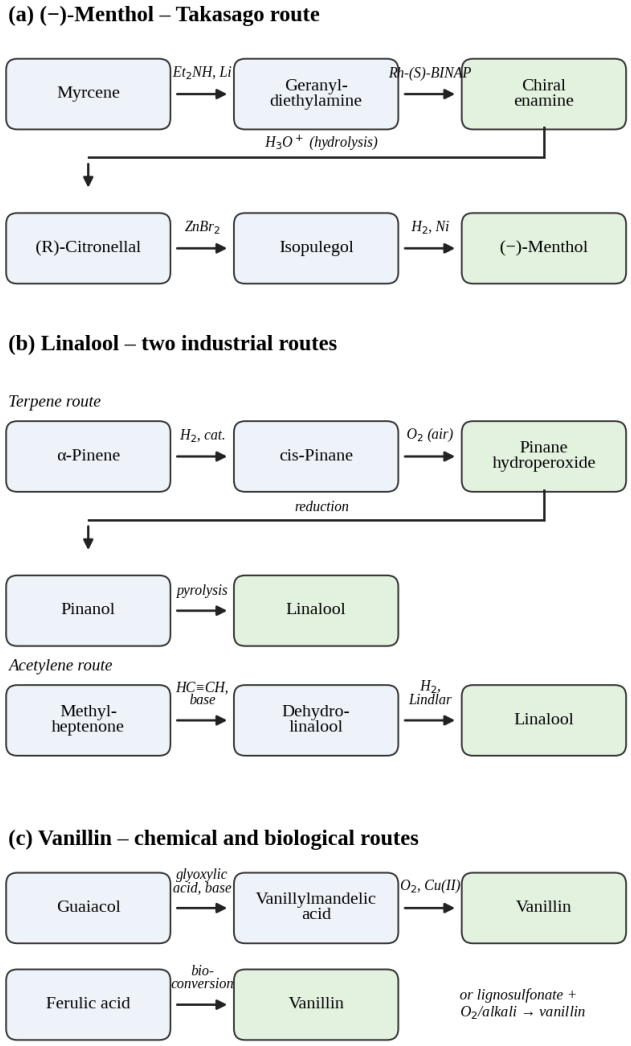


Fig. 3. Schematic synthetic sequences: (a) Takasago route to (−)-menthol; (b) two industrial routes to linalool; (c) chemical and biological routes to vanillin. Reagents are shown above the arrows; green boxes mark the final product.

A. Terpenoid Alcohols and Aldehydes

Linalool, a floral–woody tertiary alcohol, is made industrially in two ways [2]. In the terpene route, α-pinene is hydrogenated to cis-pinane, autoxidised to the hydroperoxide, reduced to pinanol and pyrolysed to open the cyclobutane ring. In the acetylene route, methylheptenone is ethynylated with acetylene under basic conditions and the resulting dehydrolinalool is hydrogenated over a poisoned (Lindlar-type) catalyst. The first route exploits renewable pinene; the second builds the skeleton from petrochemical C_2 and isoprenoid C_5 units and is closely related to vitamin intermediate chemistry. Citral is produced from prenol and prenal via an acetal that undergoes a sequence of [3,3]-sigmatropic (Claisen and Cope) rearrangements, and it is a platform for ionones and, through citronellal, for menthol [2].

(−)-Menthol is a showcase of asymmetric catalysis. In the Takasago process, myrcene is converted to a geranyl-

diethylamine, which a Rh–BINAP catalyst isomerises to a chiral enamine with very high enantioselectivity; hydrolysis gives (*R*)-citronellal, which is cyclised to isopulegol and hydrogenated to (−)-menthol [23], [24]. The work behind this process contributed to the 2001 Nobel Prize in Chemistry [24]. An alternative route hydrogenates thymol and separates the stereoisomers [2].

B. Aromatic Aldehydes, Lactones and Alcohols

Vanillin is the most widely used flavour and fragrance compound. Vanilla pods supply only a small fraction of demand [25]. Most industrial vanillin is made from guaiacol and glyoxylic acid, which condense to vanillylmandelic acid that is then oxidatively decarboxylated, and a smaller share comes from the oxidation of lignin from pulping liquors [26], [27]. "Natural" vanillin is also made by bioconversion of ferulic acid and has been studied in engineered microbes and in the vanilla orchid itself [28].

Coumarin was the first synthetic perfumery material [3]. The Perkin reaction condenses salicylaldehyde with acetic anhydride in the presence of a weak base, followed by cyclisation, and gives coumarin together with acetic acid and water as by-products. The acylating reagent is consumed, which is reflected in the low atom economy discussed below. 2-Phenylethanol, the main odorant of rose, is made by Friedel–Crafts reaction of benzene with ethylene oxide or by hydrogenation of styrene oxide; the fermentative route from L-phenylalanine through the yeast Ehrlich pathway is limited by product toxicity, which is relieved by in situ product removal [29].

C. Esters

Fruity and floral esters such as benzyl acetate and isoamyl acetate are formed by acid-catalysed (Fischer) esterification of the alcohol with the carboxylic acid, with removal of water to shift the equilibrium [11]. Solid acid resins avoid corrosive mineral acids, and immobilised lipases allow mild, solvent-free production of esters that is labelled natural when the substrates are natural [9]. Acid anhydrides give faster and irreversible reactions but release a carboxylic acid as by-product, which lowers atom economy.

D. Musks and Woody–Amber Materials

Musks illustrate the way that safety and environmental data steer synthetic chemistry. Early nitro musks were replaced by polycyclic musks such as galaxolide, made from a pentamethylindane that is hydroxyalkylated with propylene oxide and cyclised with formaldehyde. Polycyclic musks, however, were detected in aquatic environments and biota [30], which has increased interest in macrocyclic musks such as muscone and ethylene brassylate [31]. Ethylene brassylate is made from brassylic acid and ethylene glycol by oligomerisation and thermal depolymerisation to the ring. Methyl dihydrojasmonate is obtained by aldol condensation of cyclopentanone and pentanal, isomerisation, Michael addition of a malonate and decarboxylation [2], [5].

(−)-Ambrox, the key ambergris-type odorant, was long made by degrading the plant diterpene sclareol to sclareolide, reducing it to the diol and cyclising. Recent work has shown that sclareol is produced in engineered microbes [32] and that squalene-hopene cyclase converts homofarnesol directly to Ambrox [33], offering a route from sugar-derived feedstocks.

V. Biotechnological and Green Routes

Biotechnology enters fragrance manufacture at three levels [9], [34]. In biotransformation, an enzyme or whole cell converts a natural precursor to a target; examples are the oxidation of terpenes such as limonene and pinene to oxygenated flavour compounds [35] and ferulic acid to vanillin [25]. In de novo fermentation, a microorganism with a rewired pathway converts sugar into the odorant, as with 2-phenylethanol and, more recently, terpenoid precursors of amber and woody materials [32]. In biocatalytic steps within a chemical sequence, an engineered enzyme replaces a difficult chemical operation, as in the cyclisation to Ambrox [33]. Advances in enzyme discovery and engineering have broadened the scope of such steps [10], [36].

Chemical innovation continues in parallel. Lignin, a by-product of pulping and biorefining, is a renewable source of aromatic building blocks, and depolymerisation strategies that deliver vanillin and related compounds are an active area [26], [27]. Continuous-flow reactors improve heat transfer and safety for hazardous or exothermic steps such as oxidations and hydroperoxide chemistry, and have been reviewed mainly in the pharmaceutical context, where many of the same principles apply [37]. A practical limitation is the regulatory definition of "natural": a molecule labelled natural must usually derive from a natural source by physical, enzymatic or microbiological processes, so enzymatic routes add commercial value beyond sustainability alone.

VI. Comparative Assessment of Production Strategies

A. Atom Economy

Atom economy (AE) measures how much of the mass of the reactants appears in the desired product [38]:

$$\mathrm{AE}\ (\%) = [\ M_{\mathrm{product}} / \Sigma\, M_{\mathrm{reactants}}\ ] \times 100 \qquad (1)$$

where M is molar mass and the sum includes all stoichiometric reagents but not catalysts or solvents. AE is a theoretical upper bound and does not account for yield, solvent use or excess reagents. The practical waste per unit of product is described by the E factor [39]:

$$E = \text{mass of waste / mass of product} \qquad (2)$$

These two numbers are complementary, and both belong to the broader set of green-chemistry principles [40].

Fig. 4 shows AE calculated by the author from balanced equations for eight transformations. Additions and hydrogenations are inherently atom economical: ethynylation–semi-hydrogenation of methylheptenone to linalool and hydrogenation of thymol to menthol both reach 100 %. Fischer esterification gives 87.8–89.3 % because only water is lost, whereas using acetic anhydride lowers the AE of benzyl acetate to 71.4 %. The guaiacol–glyoxylic acid route to vanillin (71.0 %) and the Perkin reaction to coumarin (65.2 %) lose mass as CO_2, water and acetic acid. The 100 % value for the Friedel–Crafts reaction of benzene with ethylene oxide is misleading: it ignores the stoichiometric Lewis acid needed in practice, which dominates the waste stream and illustrates why AE and E must be read together.

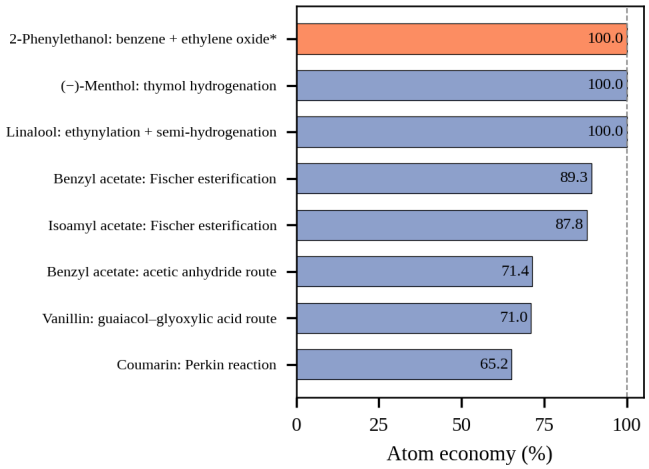


Fig. 4. Atom economy of eight representative fragrance-related transformations, calculated from balanced equations and standard atomic masses. *The benzene–ethylene oxide value excludes the stoichiometric Lewis acid actually required.

B. Qualitative Strategy Comparison

Fig. 5 scores five production strategies on five criteria on a three-point scale (3 = most favourable). The scores are the author's qualitative judgments, derived from the process descriptions and sustainability analyses cited here [2], [39], [10]; they are not measured data and refined with life-cycle inventories for specific products. Natural extraction scores well on feedstock and stereochemistry but poorly on scalability. Semisynthesis from terpene streams combines renewable carbon with mature technology. Racemic petrochemical synthesis is scalable but weak on feedstock, stereocontrol and waste. Asymmetric chemocatalysis excels in stereocontrol and scale, while biocatalysis and fermentation score highest on waste minimisation and stereoselectivity but are still limited by titres and downstream recovery. The practical conclusion is that strategies are complementary, and hybrid sequences—chemical steps from renewable terpenes combined with enzymatic selective steps—are the most promising.

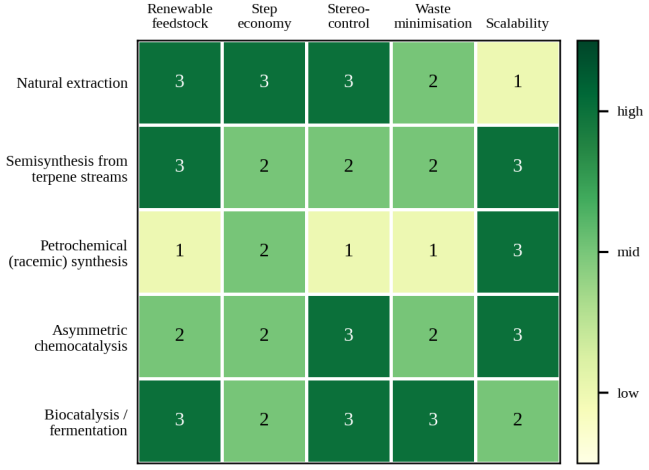


Fig. 5. Qualitative scoring (1 = low, 3 = high favourability) of five production strategies on five criteria. Scores are the author's judgment based on the cited literature and are not experimental data.

VII. Applications

Table II connects each application sector with typical materials and the property that governs the choice. In fine fragrance, odor quality, substantivity and diffusion dominate; stable base-note materials such as musks and amber compounds fix lighter components [12], [1]. In personal care and household products, the molecule must survive extremes of pH, surfactant and oxidising agents, which favours stable aromatics and macrocyclic musks over aldehydes and some esters [2]. In food and oral care, vanillin, menthol and fruity esters provide flavour and sensory effects, and purity and "natural" status are important [9].

TABLE II
Application sectors, materials and design drivers

Sector	Representative materials	Main design drivers
Fine fragrance	Linalool, methyl dihydrojasmonate, Ambrox, macrocyclic musks	Odor quality, diffusion, long-lasting base notes, allergen profile
Personal care	Citrals, 2-phenylethanol, benzyl acetate, galaxolide	Skin safety, stability in surfactants, labelling
Household	Polycyclic and macrocyclic musks, terpene alcohols	Stability at high pH, cost, biodegradability
Textiles	Microencapsulated blends of top–heart–base notes	Controlled release, wash durability, polymer shell regulation
Food and oral care	Vanillin, menthol, fruity esters	Purity, regulatory status, taste thresholds
Wellness and repellents	Linalool, citronellal, geraniol, essential oils	Efficacy evidence, volatility, safety

Encapsulation extends fragrance performance. Core–shell microcapsules protect volatile ingredients and release them on friction, heat or humidity; applied to textiles, they have given controlled release of scents through many wash cycles [41]. Because many capsule shells are synthetic polymers, the EU restriction on intentionally added polymer microparticles adopted in 2023 will push the industry toward biodegradable shells [8]. In pest control and preservation, terpenoid constituents of essential oils show repellent and antimicrobial activity, although efficacy depends strongly on dose and formulation [42], [43]. Claims for aromatherapy remain mixed: the evidence for mood and physiological effects is stronger for expectation-based than for pharmacological mechanisms [44].

VIII. Safety, Regulation and Environmental Impact

Fragrance allergens are a leading cause of cosmetic-related contact allergy, and the clinical literature has long documented sensitisation to constituents such as oxidised linalool, citral, coumarin and eugenol [45]. In the EU, the Cosmetics Regulation requires labelling of listed fragrance allergens above defined thresholds [6], and a 2023 delegated act extends the list of labelled substances [7]. Reformulation

toward less sensitising analogues, and control of hydroperoxide formation during storage, are active design goals.

Environmental considerations add further constraints. Polycyclic musks persist in sediments and bioaccumulate in aquatic biota [30], which is one reason for the shift toward macrocyclic musks [31]. For all synthetic routes, the combination of low E factor, renewable carbon and biodegradable products is becoming a requirement, not an option [39]. Microplastic regulation also applies to capsule delivery systems, as discussed above [8].

IX. Challenges and Outlook

Several research directions follow from the analysis. (1) Stereoselective catalysis for the remaining racemic commercial odorants is still incomplete, and enzymes and earth-abundant metal catalysts could replace precious-metal systems [36], [24]. (2) Fermentation titres and downstream recovery for volatile and toxic products need to improve to compete with petrochemical cost [29], [34]. (3) Lignin and other biomass streams require selective, scalable depolymerisation to deliver pure aromatic aldehydes [27]. (4) Data-driven odor models are linked with synthesis planning, so that molecules with target odor and good safety and biodegradability is designed and prioritised before synthesis [16], [17]. (5) Life-cycle assessment of natural, nature-identical and biotechnological versions of the same molecule is needed to replace qualitative arguments such as those in Fig. 5. (6) Biodegradable capsule shells with equivalent performance are urgently needed for delivery systems [8], [41]. Continuous-flow processing is likely to support several of these developments by making hazardous oxidations and hydrogenations safer and easier to scale [37].

X. Conclusion

Fragrance synthesis has moved from the first preparation of coumarin to a broad toolbox of asymmetric catalysis, renewable-feedstock semisynthesis, biocatalysis and fermentation. A volatility analysis connects the physical properties of the main odorants to the perfume pyramid, atom-economy calculations show that catalytic additions and hydrogenations are much more mass-efficient than condensations and acylations, and a qualitative comparison indicates that biocatalysis and asymmetric catalysis complement rather than replace each other. The next stage of progress will come from hybrid chemoenzymatic sequences from renewable terpenes and lignin, from safer low-allergen molecules designed with predictive odor models, and from biodegradable delivery systems that comply with emerging regulation.

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